Claims

[c1] 1. A method to improve a CHTS experiment, comprising steps of:

formulating an array of a mixture of at least two components;

conducting an experiment on the array to produce results; and

applying at least one Six Sigma technique to a step of the experiment to improve results of the experiment.

[c2] 2. The method of claim 1, additionally comprising monitoring the step of formulating the array of a mixture.

[c3] 3. The method of claim 1, additionally comprising monitoring the step of formulating the array of a mixture and identifying the step as an opportunity for a defect.

[c4] 4. The method of claim 1, wherein the array of a mixture is formulated by delivering components of reactants to a well of an array plate.

[c5] 5. The method of claim 1, wherein the array of a mixture is formulated by delivering components of reactants to a well of an array plate using a robotic dispenser.

[c6] 6. The method of claim 1, wherein applying at least one Six Sigma technique includes identifying a defect opportunity.

[c7] 7. The method of claim 1, wherein applying at least one Six Sigma technique includes identifying a defect opportunity selected from steps of monitoring a stock precursor solution, mixing an aliquot of the stock solution with an aliquot of another solution, delivering a mixture of the aliquots to a well of an array plate, effecting a condition of reaction on the mixture, detecting a result of the reaction and analyzing the result to determine either a lead or to determine a candidate library for reiterating the experiment.

[c8] 8. The method of claim 1, comprising (A) an iteration of steps of (i) formulating an array of mixtures of at least two components; (ii) reacting the array mixtures; and (iii) evaluating a set of products of the reacting step and

(B) repeating the iteration of steps (i), (ii) and (iii) wherein components of a successive array of mixtures selected for a step (i) are chosen as a result of an evaluating step (iii) of a preceding iteration.

[c9] 9. The method of claim 1, wherein applying the Six Sigma technique comprises determining a Sigma value as equal to an absolute value function of a difference between average value of measurements on the system minus a nearest specification divided by a standard deviation of the measurements on the system.

[c10] 10. The method of claim 1, wherein applying the Six Sigma technique comprises determining a Sigma value as equal to per million occurrences of a ratio of number of defects of a product to number of opportunities for defect times number of units of the product.

[c11] 11. The method of claim 1, wherein applying at least one Six Sigma technique includes identifying a step of delivering stock solution to a well or substrate as a critical to quality defect opportunity.

[c12] 12. The method of claim 1, wherein applying at least one Six Sigma technique includes identifying a defect as a ternary mixture concentration that deviates more than ($l/3^* \sqrt{\ } 3$) from a design concentration where l is a height of an equilateral triangle of a graphic representation of the mixture.

[c13] 13. The method of claim 1, wherein applying at least one Six Sigma technique includes calculating a Sigma value equal to ($l/3^* \sqrt{\ } 3)/_{P}$ where l is a height of an equilateral triangle of a graphic representation of the mixture and $_{P}$ is standard deviation.

[c14] 14. The method of claim 1, wherein the Six Sigma technique includes establishing a project goal Sigma value of at least 4.5.

[c15] 15. The method of claim 1, wherein the Six Sigma technique includes establishing a project goal Sigma value of at least 5.0.

[c16] 16. The method of claim 1, wherein the Six Sigma technique includes

establishing a project goal Sigma value of at least 5.5.

[c17] 17. The method of claim 1, wherein the Six Sigma technique includes (1) selecting a point on a gradient representation of the mixture; (2) selecting a design concentration for each stock solution and an estimate of the standard deviation for each stock solution used to generate a mixture represented by the point; (3) determining an amount of each stock solution required to generate the mixture; (4) randomly selecting another stock concentration value from normal value distributions of concentration from the point mixture; (5) calculating a delivered concentration of components of a mixture resulting from mixing design amounts of stock solution; (6) calculating a distance between delivered concentration and the design concentration; and (7) counting a defect when the calculated distance exceeds I/3* $\sqrt{}$ 3.

[c18] 18. The method of claim 17, wherein steps (3) to (7) are repeated until at least 3 defects are counted.

[c19] 19. The method of claim 17, wherein steps (3) to (7) are repeated until at least 10 defects are counted.

[c20] 20. The method of claim 17, wherein steps (3) to (7) are repeated until 1,000,000 defect opportunities are counted.

[c21] 21. The method of claim 17, wherein the mixture is a ternary, quaternary or pentanary mixture.

[c22] 22. The method of claim 17, wherein steps (3) and (4) are determined according to formulas (III) through (VII) based on an assumption of no error in the stock solution concentration.

[c23] 23. The method of claim 17, wherein the distance between delivered concentration and design concentration is calculated according to the formula (where SQRT is the square root function).

[c24] 24. The method of claim 1, wherein the Six Sigma technique identifies at

least one of viscosity of stock solution, speed of withdrawal of solution from a stock solution vial, speed of addition to an array well and diameter of pipet tip as an area for improving Sigma of the formulating step.

[c25] 25. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities.

[c26] 26. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value.

[c27] 27. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value by comparing the ratio to a Sigma chart.

[c28] 28. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value by comparing the ratio to a Sigma chart stored in the data base of a processor.

[c29] 29. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value corresponding to defects per million opportunities (DPMO).

[c30] 30. The method of claim 1, wherein a low Sigma cause is identified and Sigma is improved by improving the low sigma cause.

[c31] 31. The method of claim 1, wherein the components include a catalyst system comprising combinations of Group IVB, Group VIB and Lanthanide Group metal complexes.

[c32] 32. The method of claim 1, wherein the components include a catalyst system comprising a Group VIII B metal.

[c33]

33. The method of claim 1, wherein the components include a catalyst

system comprising palladium.

[c34] 34. The method of claim 1, wherein the components include a catalyst system comprising a halide composition.

[c35] 35. The method of claim 1, wherein the components include an inorganic co-catalyst.

[c36] 36. The method of claim 1, wherein the components include a catalyst system that includes a combination of inorganic co-catalysts.

[c37] 37. A method, comprising:

identifying a reactant delivering step as an opportunity for a defect in a CHTS experiment;

measuring a number of units produced by the delivering step;

measuring defects in the units produced by the delivering step of the repeated CHTS; and

calculating a defects per unit for the delivering step.

[c38] 38. The method of claim 37, wherein the CHTS experiment comprises an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating products after completion of a single or repeated iteration.

[c39] 39. The method of claim 37, wherein the CHTS experiment comprises effecting parallel chemical reactions of an array of reactant mixtures.

[c40] 40. The method of claim 37, wherein the CHTS experiment is characterized by parallel reactions at a micro scale.

[c41] 41. The method of claim 37, wherein the CHTS experiment comprises (A) an iteration of steps of (i) delivering mixtures of reactants to array wells; (ii) reacting the mixtures and (iii) evaluating a set of products of the reacting step and (B) repeating the iteration of steps (i), (ii) and (iii) wherein a successive mixture of reactants selected for a step (i) is chosen as a result of an evaluating step (iii) of a preceding iteration.

[c42] 42. The method of claim 37, wherein the CHTS experiment comprises effecting parallel chemical reactions of an array of ternary reactant mixtures.

[c43] 43. A method, comprising:

identifying a reactant delivering step or stock formulating step as an opportunity for a defect in a mixture experiment;

measuring a number of units produced by the delivering step or formulating step;

measuring defects in the units produced by the delivering step or the formulating step; and

calculating a defects per unit for the delivering step or formulating step.

[c44] 44. The method of claim 43, wherein the experiment is a ternary, quaternary or pentanary mixture experiment.

[c45] 45. The method of claim 43, wherein the experiment is a ternary, mixture experiment.